Open-Volume Microstructural Analysis

Polymer free-volume analysis and semiconductor materials analysis

Elastic and electrical properties, impact strength, and aging are qualities that determine the commercial utility of polymers. These qualities can be understood using a unifying theory based on the free molecular volume of the material. Application of this theory, however, has been limited by a lack of definitive measurements. A new method—positron annihilation spectroscopy (PAS)—can directly measure, through the positron lifetime, the microscopic free-volume fraction and size distribution in a nondestructive setting. With PAS, we can determine the number and size of free volume elements from 1 to over 2000 Å^3.

Semiconductor materials analysis

Electrical properties of semiconducting materials and devices are determined by defects either purposefully introduced or accidentally occurring. Nondestructive analysis of defects is important for quality assurance in the bulk and particularly at interfaces in layers deposited for device fabrication. We have successfully conducted in-bulk PAS experiments specific to defect type and charge state in semiconductors.

We can use monoenergetic positrons to measure the depth distribution and microscopic characteristics of defects in semiconducting materials and structures. These measurements can be related to the charge carrier diffusion, interfacial defect concentrations, and defect population of thin-layered materials.

APPLICATIONS

- *Characterization of defects in semiconductor materials*
- *Aging of fiber composites*
- *High-temperature superconductor materials*
- *Polymer thin films*
- *Radiation-damaged materials*

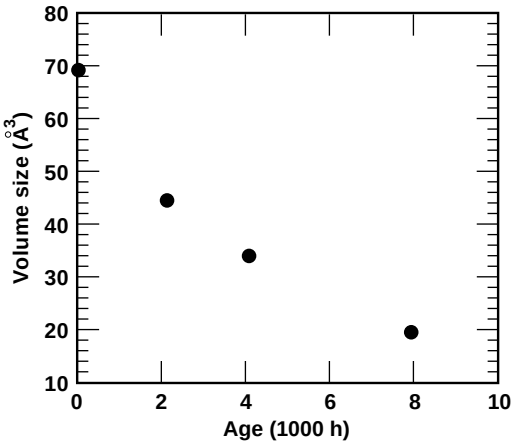
Current LLNL capabilities

We can perform all major PAS experiments—we pioneered intense positron beams and angular correlation spectrometers that are now copied worldwide.

Our experimental work has produced valuable data on the behavior of materials systems:

- Defect determinations
- Unique demonstrations of the Fermi surface in high-temperature superconductors
- Original studies on the value of positron spectroscopy as a surface electronic structure probe.

We can determine the free volume in thick samples of polymeric materials in situ under set conditions of temperature, pressure, and mechanical stress.



PAS can nondestructively characterize the effects of aging in lightweight materials and fiber composites.

Emerging capabilities

A pulsed, monoenergetic beam of positrons that can be implanted in the film material is necessary to measure the free volume in free-standing thin films and coatings and identify semiconductor defects in deposited layers and at interfaces. By developing a positron-pulsed beam microprobe, we are creating the only U.S. facility capable of measuring the depth dependence, spatial distribution, and specific identity of free volume and defect populations.

Availability: We are seeking industrial partners with whom we can share our bulk- or thin-film capabilities. We also seek industrial partners to develop new thin-film techniques for specific applications.

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